

What is claimed is:

1. A crystallized P-selectin LE.
- 5 2. The crystallized P-selectin LE of Claim 1, characterized as being in plate form with space group  $P2_1$ , and having unit cell parameters of  $a=81.0\text{\AA}$ ,  $b=60.8\text{\AA}$ ,  $c=91.4\text{\AA}$ , and  $\beta=103.6^\circ$ .
- 10 3. A crystallized complex of P-selectin LE and  $\text{SLe}^x$ .
4. The crystallized complex of Claim 3, characterized as being in plate form with space group  $P2_1$ , and having unit cell parameters of  $a=81.1\text{\AA}$ ,  $b=60.5\text{\AA}$ ,  $c=91.4\text{\AA}$ , and  $\beta=103.3^\circ$ .
- 15 5. A crystallized complex of E-selectin LE and  $\text{SLe}^x$ .
6. The crystallized complex of Claim 5, characterized as being in rod form with space group  $P2_12_12_1$ , and having unit cell parameters of  $a=34.5\text{\AA}$ ,  $b=72.4\text{\AA}$ , and  $c=77.6\text{\AA}$ .
- 20 7. A crystallized complex of P-selectin LE and a PSGL-1 peptide.
8. The crystallized complex of Claim 7, characterized as being in bipyramidal form with space group  $I222$  and having unit cell parameters of  $a=63.4\text{\AA}$ ,  $b=96.8\text{\AA}$ , and  $c=187.3\text{\AA}$ .
- 25 9. An active site of an  $\text{SLe}^x$  binding protein or peptide, wherein said active site comprises the relative structural coordinates of amino acid residues TYR48, GLU80, ASN82, GLU92, TYR94, PRO98, SER99, ASN105,

ASP106, GLU107 and bound calcium according to Figure 3,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

5                    10.    The active site of Claim 9, wherein said active site further comprises the relative structural coordinates of amino acid residues TYR44, SER46, SER47, ALA77, ASP78, ASN79, PRO81, ASN83, ARG85, GLU88, CYS90, ILE93, LYS96, SER97, ALA100, TRP104, HIS108, LYS111 and LYS113 according to Figure 3,  $\pm$  a root mean square deviation from the backbone atoms  
10 of said amino acids of not more than 1.5Å.

15                    11.    An active site of an SLe<sup>x</sup> binding protein or peptide, wherein said active site comprises the relative structural coordinates of amino acid residues TYR48, GLU80, ASN82, ASN83, GLU92, TYR94, ARG97, GLU98, ASN105, ASP106, GLU107 and bound calcium according to Figure 4,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

20                    12.    The active site of Claim 11, wherein said active site further comprises the relative structural coordinates of amino acid residues TYR44, SER45, PRO46, SER47, ALA77, PRO78, GLY79, PRO81, GLU88, CYS90, LYS99, ASP100, TRP104, ARG108, LYS111 and LYS113 according to Figure 4,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

25                    13.    An active site of a PSGL-1 binding protein or peptide, wherein said active site comprises the relative structural coordinates of amino acid residues ALA9, TYR45, SER46, SER47, TYR48, GLU80, ASN82, LYS84, ARG85, GLU88, GLU92, TYR94, PRO98, SER99, ASN105, ASP106, GLU107,  
30 HIS108, LEU110, LYS111, LYS112, LYS113, HIS114 and bound strontium

according to Figure 5,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

14. The active site of Claim 13, wherein said active site further  
5 comprises the relative structural coordinates of amino acid residues SER6, THR7, LYS8, TYR10, SER11, TYR44, TYR49, TRP50, ALA77, ASP78, ASN79, PRO81, ASN83, ASN86, ASN87, CYS90, ILE93, ILE95, LYS96, SER97, ALA100, TRP104 and CYS109 according to Figure 5,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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15. A method for identifying an agent that interacts with P-selectin LE, comprising the steps of:

(a) generating a three dimensional model of P-selectin LE using the relative structural coordinates according to Figures 2, 3 or 5,  $\pm$  a root mean  
15 square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and

(b) employing said three-dimensional model to design or select an agent that interacts with P-selectin LE.

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16. The method of Claim 15, further comprising the steps of:  
(c) obtaining the identified agent; and (d) contacting the identified agent with P-selectin LE in order to determine the effect the agent has on P-selectin LE activity.

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17. A method for identifying an activator or inhibitor of a molecule or molecular complex comprising an SLe<sup>x</sup> binding site, comprising the steps of:

(a) generating a three dimensional model of said molecule or molecular complex comprising an SLe<sup>x</sup> binding site using (i) the relative  
30 structural coordinates according to Figure 3 of residues TYR48, GLU80, ASN82,

GLU92, TYR94, PRO98, SER99, ASN105, ASP106, GLU107 and bound calcium,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than  $1.5\text{\AA}$ , or (ii) the relative structural coordinates according to Figure 4 of amino acid residues TYR48, GLU80, ASN82, GLU92, TYR94, ARG97, GLU98, ASN105, ASP106, GLU107 and bound calcium,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than  $1.5\text{\AA}$ ; and

- (b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis of the candidate activator or inhibitor with the three dimensional model generated in step (a).

18. The method of Claim 17, wherein the relative structural coordinates according to Figure 3 further comprises amino acid residues TYR44, SER46, SER47, ALA77, ASP78, ASN79, PRO81, ASN83, ARG85, GLU88, CYS90, ILE93, LYS96, SER97, ALA100, TRP104, HIS108, LYS111 and LYS113,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than  $1.5\text{\AA}$ .

19. The method of Claim 17, wherein the relative structural coordinates according to Figure 4 further comprises the amino acid residues TYR44, SER45, PRO46, SER47, ALA77, PRO78, GLY79, PRO81, GLU88, CYS90, LYS99, ASP100, TRP104, ARG108, LYS111 and LYS113,  $\pm$  a root mean square deviation from the backbone atoms of said amino acids of not more than  $1.5\text{\AA}$ .

20. The method of Claim 17, which further comprises the steps of: (c) obtaining the candidate activator or inhibitor; and (d) contacting the candidate activator or inhibitor with the molecule or molecular complex and determining the effect the candidate activator or inhibitor has on the molecule or molecular complex.

21. The method of Claim 20, wherein the candidate activator or inhibitor is contacted with the molecule or molecule complex in the presence of SLe<sup>x</sup> in order to determine the effect the candidate activator or inhibitor has on binding of the molecule or molecular complex to SLe<sup>x</sup>.

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22. A method for identifying an activator or inhibitor of a molecule or molecular complex comprising a PSGL-1 binding site, comprising the steps of:

(a) generating a three dimensional model of said molecule or  
10 molecular complex comprising a PSGL-1 binding site using the relative structural coordinates according to Figure 5 of amino acid residues ALA9, TYR45, SER46, SER47, TYR48, GLU80, ASN82, LYS84, ARG85, GLU88, GLU92, TYR94, PRO98, SER99, ASN105, ASP106, GLU107, HIS108, LEU110, LYS111, LYS112, LYS113, HIS114 and bound strontium,  $\pm$  a root mean square deviation  
15 from the backbone atoms of said amino acids of not more than 1.5Å; and

(b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis of the candidate activator or inhibitor with the three dimensional model generated in step (a).

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23. The method of Claim 22, wherein the relative structural coordinates according to Figure 5 further comprises amino acid residues SER6, THR7, LYS8, TYR10, SER11, TYR44, TYR49, TRP50, ALA77, ASP78, ASN79, PRO81, ASN83, ASN86, ASN87, CYS90, ILE93, ILE95, LYS96, SER97, ALA100, TRP104 and CYS109,  $\pm$  a root mean square deviation from the backbone atoms  
25 of said amino acids of not more than 1.5Å.

24. The method of Claim 22, which further comprises the steps of: (c) obtaining the candidate activator or inhibitor; and (d) contacting the candidate activator or inhibitor with the molecule or molecular complex and

determining the effect the candidate activator or inhibitor has on the molecule or molecular complex.

25. The method of Claim 24, wherein the candidate activator or  
5 inhibitor is contacted with the molecule or molecule complex in the presence of  
PSGL-1 or a PSGL-1 peptide in order to determine the effect the candidate  
activator or inhibitor has on binding of the molecule or molecular complex to  
PSGL-1 or a PSGL-1 peptide.

10 26. A method for identifying an agent that interacts with  $SLe^x$ ,  
comprising the steps of:

- (a) generating a three dimensional model of  $SLe^x$  using the  
relative structural coordinates according to Figures 3 or 4,  $\pm$  a root mean square  
deviation from the backbone atoms of said amino acids of not more than  $1.5\text{\AA}$ ;  
15 and  
(b) employing said three-dimensional structure to design or  
select an agent that interacts with  $SLe^x$ .

27. The method of Claim 26, further comprising the steps of:  
20 (c) obtaining the identified agent; and (d) contacting the identified agent with  
 $SLe^x$  in order to determine the effect the agent has on  $SLe^x$  activity.

28. A method for identifying an agent that interacts with PSGL-  
1, comprising the steps of:

- 25 (a) generating a three dimensional model of a PSGL-1 peptide  
using the relative structural coordinates according to Figure 5,  $\pm$  a root mean  
square deviation from the backbone atoms of said amino acids of not more than  
 $1.5\text{\AA}$ ; and  
(b) employing said three-dimensional structure to design or  
30 select an agent that interacts with PSGL-1.

29. The method of Claim 28, further comprising the steps of:  
(c) obtaining the identified agent; and (d) contacting the identified agent with  
PSGL-1 or a PSGL-1 peptide in order to determine the effect the agent has on  
PSGL-1 or the PSGL-1 peptide activity.

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30. An agent identified by the method of Claim 15.

31. An inhibitor or activator identified by the method of Claim  
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32. An inhibitor or activator identified by the method of Claim  
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33. An agent identified by the method of Claim 26.

34. An agent identified by the method of Claim 28.

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35. A method for obtaining a crystallized complex of an E-  
selectin type molecule and a compound that coordinates calcium, said method  
comprising the steps of:

(a) contacting a crystallized E-selectin type molecule with a  
compound that coordinates calcium in the presence of calcium ions and PEG to  
form a crystallized complex of the E-selectin type molecule and said compound  
that coordinates calcium; and

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(b) contacting said crystallized complex in the presence of a  
reduced concentration of calcium ions, and sufficient concentrations of PEG and  
an ionic salt to obtain a final crystallized complex, that upon cooling, is suitable  
for elucidating the three dimensional structures of the E-selectin type molecule  
and said compound that coordinates calcium by x-ray diffraction of said final  
30 crystallized complex.